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Note on starting the Numerov method more accurately by a hybrid formula of order four for an initial—value problem

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Abstract

In this note we report a hybrid formula of order four for starting the Numerov method applied to the initial—value problem for $y'' = f(x, y)$, over the recently obtained result of order three by two different papers (J. Pure Appl. Sci. 2(2) (2002) 1, Abacus 29(2) (2002) 92), based on two different approaches. We illustrate the accuracy of the methods by two numerical examples.

1. Introduction

Let us consider the solution of the special second order ordinary differential equation

$$y'' = f(x, y), \quad y(a) = y_0, \quad y'(a) = y'_0, \tag{1.1}$$

where $a \leqslant x \leqslant b$. The three-term recurrence formula

$$y_{r+2} - 2y_{r+1} + y_r = \frac{h_r^2}{12}(f_{r+2} + 10f_{r+1} + f_r) \tag{1.2}$$

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is called the Numerov method for efficient solution of (1.1) on a discrete mesh point with variable step-size h_r of the form

$$x_{r+1} = x_r + h_r, \quad r = 0, 1, \ldots, n-2, \qquad x_n = x_{n-1} + h_{n-1}, \tag{1.3}$$

where $a = x_0, x_r < x_{r+1}, r = 1, \ldots, n-1, x_n = b$.

The formula (1.2) is accurate of order four with an error term whose coefficient $c_6 = -1/240$. Its application to (1.1) results in a tridiagonal set of algebraic equations. For these two reasons the Numerov method is popular. A parallel algorithm designed to speed up the calculation with (1.2) was proposed in Yusuph and Onumanyi [4] and further developed by Onumanyi et al. [2]. Whether for parallel or sequential computation the issue of starting with the Numerov method accurately has important consequence on the global error of the general algorithm (see Tables 3.1(b) and 3.2(b) in section three of this note).

For this reason Gonzalez and Thompson [1] obtained using Taylor series approach a starting formula

$$y_1 = y_0 + h_0 y_0' + \frac{h_0^2}{24}\left(7f_0 + 6f_1 - f_2\right), \tag{1.4}$$

where (1.4) has a global error $o(h_r^3)$.Yusuph and Onumanyi [4] using multistep collocation approach obtained the same formula (1.4).

In this note, a more accurate starting formula (hybrid method) with global error $o(h_r^4)$ based on the multistep collocation approach is reported as a replacement for (1.4). This is shown in Section 2 while Section 3 gives two numerical examples to compare the methods for accuracy.

2. A method of order four $o(h_r^4)$

Let us state here the parallel algorithm proposed by Yusuph and Onumanyi [4] and Onumanyi et al. [2].

Step one: For $r = 0$, solve (1.1) by (1.2) and (1.4) simultaneously for the first point y_1 and the second point y_2 of the solution on the mesh points $\{x_0, x_1, x_2\}$. In this case $h_0 = x_1 - x_0 = x_2 - x_1 = h$, fixed step.

Step $r > 0 : r = 2, 4, \ldots, n$: Solve for each value of r simultaneously, equations

(i) (1.2) and (ii)

$$y_{r-1} - 2y_r + y_{r+1} = -\frac{h_r^2}{24}(f_{r-2} - 6f_{r-1} - 14f_r - 6f_{r+1} + f_{r+2}). \tag{2.1}$$

Comment (1.1)

The formula (2.1) ensures continuity of the first derivative function obtained by a continuous interpolant from the multistep collocation. Formula (2.1) has a global error $o(h_r^4)$ and $c_6 = 3/80$. We see that the step one of the above algorithms is accurate of order $\binom{4}{3}$ while the subsequent steps $r > 0$ are accurate of order $\binom{4}{4}$.

Following a multistep collocation approach, Sirisena and Onumanyi [3] developed a continuous interpolant valid in $[x_r, x_{r+2}]$ of the form

$$\begin{aligned} y(\zeta) =& \phi_0(\zeta)y_r + \phi_1(\zeta)y_{r+1} + \phi_{3/2}(\zeta)y_{r+3/2} + \psi_0(\zeta)f_r \\ &+ \psi_0(\zeta)f_r + \psi_1(\zeta)f_{r+1} + \psi_2(\zeta)f_{r+2}, \end{aligned} \tag{2.2}$$

where $\zeta := (x - x_r)$,

$$\phi_0(\zeta) = \frac{1}{75h^5}\left(48\zeta^5 - 240h\zeta^4 + 320h^2\zeta^3 - 203h^4\zeta + 75h^5\right),$$

$$\phi_1(\zeta) = \frac{1}{25h^5}\left(-48\zeta^5 + 240h\zeta^4 - 320h^2\zeta^3 + 153h^4\zeta\right),$$

$$\phi_{3/2}(\zeta) = \frac{1}{75h^5}\left(96\zeta^5 - 480h\zeta^4 + 640h^2\zeta^3 - 256h^4\zeta\right),$$

$$\psi_0(\zeta) = \frac{1}{600h^3}\left(-42\zeta^5 + 235h\zeta^4 - 430h^2\zeta^3 + 300h^3\zeta^2 - 63h^4\zeta\right),$$

$$\psi_1(\zeta) = \frac{1}{300h^3}\left(-126\zeta^5 + 605h\zeta^4 - 740h^2\zeta^3 + 261h^4\zeta\right),$$

$$\psi_2(\zeta) = \frac{1}{600h^3}\left(6\zeta^5 - 5h\zeta^4 - 10h^2\zeta^3 + 9h^4\zeta\right),$$

was developed in [4].

The evaluation of (2.2) at $x = x_{r+2}$ yields (1.2) while collocation at $x = x_{r+3/2}$ gives

$$y_{r+3/2} - \frac{3}{2}y_{r+1} + \frac{1}{2}y_r = \frac{h_r^2}{96}\left(3f_{r+2} - 10f_{r+3/2} + 39f_{r+1} + 4f_r\right). \tag{2.3}$$

At $x = x_r$, the first derivative of (2.2) gives

$$\frac{256}{75}y_{r+3/2} - \frac{153}{25}y_{r+1} + \frac{203}{75}y_r + h_r y_r' = \frac{h_r^2}{600}\left(9f_{r+2} + 522f_{r+1} - 63f_r\right). \tag{2.4}$$

Eqs. (1.2), (2.3) and (2.4) constitute the members of a zero—stable block integrator of order four with $c6 = \begin{pmatrix} -\frac{1}{240} \\ -\frac{21}{10240} \\ -\frac{3}{4000} \end{pmatrix}$. The application of the block integrator with $r = 0$ gives the accurate values of y_1, y_2 along with $y_{3/2}$ as shown in tables of Section 3. However, the accurate values obtained using (1.2), (2.3) and (2.4) can be equivalent to the theoretical one (1.2) and (2.6). Substituting the expression for $y_{r+3/2}$ obtained from (2.3) into (2.4) gives

$$y_{r+1} - y_r - h_r y_r' = \frac{h_r^2}{360}\left(33f_{r+2} - 128f_{r+3/2} + 186f_{r+1} + 89f_r\right). \tag{2.5}$$

For $r = 0$ in (2.5) we get

$$y_1 - y_0 - h_0 y_0' = \frac{h_0^2}{360}\left(33f_2 - 128f_{3/2} + 186f_1 + 89f_0\right) \tag{2.6}$$

of global error $o(h_0^4)$ with $c_6 = -1/160$.

Table 3.1(a)
Absolute errors for example 3.1

x	Combined (2.3) and (2.4) (see also [3])	(2.6)	(1.4)
0.00	0.00	0.00	0.00
0.10	6.92 (−9)	6.92 (−9)	2.02 (−7)
0.15	1.24 (−8)	1.24 (−8)	—
0.20	1.76 (−8)	1.76 (−8)	4.07 (−7)

Starting values are provided for (1.2) by three different formulae.

Table 3.1(b)
Absolute errors for example 3.2

x	Combined (2.3) and (2.4) (see also [3])	(2.6)	(1.4)
0.000	0.00 (0)	0.00 (0)	0.00 (0)
0.010	4.96 (−9)	4.96 (−9)	2.04 (−7)
0.015	9.57 (−9)	9.57 (−9)	—
0.020	1.49 (−8)	1.49 (−8)	4.15 (−7)

Starting values are provided for (1.2) by three different formulae.

Eq. (2.8) is our new result of this note to start (1.2). In using the combination of (1.2) and (2.6) in the examples that follow, $y_{3/2}$ is estimated from what was obtained by (1.2), (2.3) and (2.4) for fair comparison with (1.4).

3. Numerical examples

Example 3.1: Solve $y'' + y = 0$, $0 \leqslant x \leqslant 0.2$, $y(0) = 1 = y'(0)$, $h_0 = h = 0.1$ [Exact solution $y(x) = \cos x + \sin x$].

Example 3.2: Solve $y'' - 100y = 0$, $0 \leqslant x \leqslant 0.02$, $y(0) = 1$, $y'(0) = -10$, $h_0 = h = 0.01$ [Exact solution $y(x) = \exp(-10x)$].

The results of Tables 3.1(a) and 3.2(a) show that:

(i) The combined application of (2.3) and (2.4) leads to the same accuracy with (2.6) numerically. This has been shown in section two. In practice, we start (1.2) with (2.4) either for parallel computation as shown or for sequential computation as in [1]. The use of (2.3) and (2.4) is equivalent to using an order for hybrid formula (2.6) to start (1.2).

(ii) The results obtained by (2.6) or equivalently by (2.3) and (2.4) combined are more accurate than those obtained by (1.4).

The results of Tables 3.1(b) and 3.2(b) that follow next show the effect of the accuracy of the starting formula on the global error of (1.2) for parallel computation as demonstrated with (2.1), the stable Numerov block method (see also [2]).

Note: In Tables 3 above, $a(b) := a \times 10^b$.

Table 3.2(a)
Solution of example 3.1 for $r \geqslant 1$ in (1.2)

x	(2.6)	(1.4)
0.3	1.62 (−8)	6.12 (−7)
0.4	4.37 (−8)	8.17 (−7)
0.5	1.20 (−7)	1.02 (−6)
0.6	1.87 (−7)	1.22 (−6)
0.7	3.07 (−7)	1.41 (−6)
0.8	4.19 (−7)	1.60 (−6)
0.9	5.79 (−7)	1.76 (−6)
1.0	7.27 (−7)	1.92 (−6)
1.1	9.20 (−7)	2.07 (−6)
1.2	1.10 (−6)	2.20 (−6)

A comparison of the global absolute errors of (1.2), starting with (2.6) or (1.4). These calculations were done using (2.1), the stable Numerov block method (see [2]).

Table 3.2(b)
Solution of example 3.2 for $r \geqslant 1$ in (1.2)

x	(2.6)	(1.4)
0.03	6.68 (−9)	6.33 (−7)
0.04	2.40 (−8)	8.61 (−7)
0.05	6.77 (−7)	1.10 (−6)
0.06	1.08 (−7)	1.35 (−6)
0.07	1.77 (−7)	1.62 (−6)
0.08	2.32 (−7)	1.91 (−6)
0.09	3.13 (−7)	2.22 (−6)
0.10	3.95 (−7)	2.56 (−6)
0.11	4.96 (−7)	2.92 (−6)
0.12	6.00 (−6)	3.31 (−6)

A comparison of the global absolute errors of (1.2), starting with (2.6) or (1.4). These calculations were done using (2.1), the stable Numerov block method (see [2]).

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